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THRESHOLD BEHAVIOR OF IONIZATION CROSS SECTIONS

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INTRODUCTION AND SUMMARY

The behavior of the ionization cross section near the threshold is determined by the interaction of particles at great distances. If the forces between all three particles flying apart are short-range forces, then $\sigma_{ioniz} \sim E^2$ [1]. If, on the other hand, two of the particles are attracted to each other according to Coulomb's law and interact with the third one by means of short-range forces, then $\sigma_{ioniz} \sim E^{\frac{3}{2}}$ [2]. Assuming that the interaction force between two particles flying apart is a short-range force and that the attraction of both particles to the third one is a Coulomb force, we obtain $\sigma_{ioniz} \sim E$ [3].

Of great practical importance in the theory of electron-atomic collisions is the case when 2 particles (electrons) repel each other and are attracted to a third particle (ion) by Coulomb forces. In this case, various and insufficiently accurate approximations yield greatly differing results. Thus, in a Born approximation $\sigma_{ioniz} \sim E^{\frac{3}{2}}$, while in a Coulomb-Born approximation $\sigma_{ioniz} \sim E$. More precise calculations [4,5] also yield one of these rules depending upon which part of the Coulomb interaction is taken into account with greater precision. These differences show that in order to obtain a correct threshold dependence it is necessary to accurately account for all Coulomb interactions, none of which being considered as short-range interaction. One such method of calculation was proposed by Wannier [6], who found that the total ionization cross section of a neutral atom is proportional to $E^{1.127}$.

Experimental results [7] also indicate small deviations from linearity.

In this article, the angular and energy distribution of electrons escaping after ionization is investigated near the threshold by the Wannier's method. In the first section, a brief

* Rasseyaniye Elektronov na Atomakh

description is given of Wannier's method in a slightly modified form, from which it follows that, in the case of small energies, electrons escape in most cases after ionization into nearly opposite directions, i.e. with $\vartheta_{12} - \pi \ll 1$. Further, it is shown that, as the energy decreases, the dependence of the complementary angular distribution on $\vartheta_{12} - \pi$ remains similar and that only the distribution width decreases proportionally to $E^{\frac{1}{4}}$, if the charge of the remaining ion Z is equal to 1 or 2 & $E^{\frac{1}{4}-\frac{\nu}{2}}\left(0 < \nu < \frac{1}{2}\right)$ and at higher values of Z.

The energy distribution of escaping electrons was also investigated. For this purpose, a numerical integration of the differential equations of motion was carried out. It was found that the probability density dw/dE_1 is practically independent of the distribution of energies E_1 and E_2 between electrons (when Z=1 in the entire ionization range the probability density varies within a 1% range). In order to find the reasons for this rule, a study was made of the case when the interaction potentials are inversely proportional to the squares of distances. Such a potential is not found in nature, but, as Jacobi has shown [8], the equations of motion admit in this case an analytical solution. It was found that the probability density also remains practically constant in this case (when Z=1 in the entire ionization range, deviations do not exceed 1% either).

THE WANNIER'S THEORY

First, let us briefly examine, from a qualitative view point, the process of single ionization at energies close to threshold.

Following a collision, two electrons escape from the atom at a certain angle with rather high velocities. As the distances, $\mathbf{r}_1$ and $\mathbf{r}_2$, from these electrons to the remaining ion increase, their velocities decrease since the electrons must overcome the attractive force of the ion. As a result of the repulsion of the electrons, the angle ϑ_{12}, between their radii increases, approaching π. This process goes on until the interaction energy $U(\mathbf{r}_1, \mathbf{r}_2)$ as $\mathbf{r}_1$ and $\mathbf{r}_2$ increase becomes considerably lower than the total energy E.

$$|U(\mathbf{r}_1, \mathbf{r}_2)| \ll E. \qquad (1)$$

Further, each of the two electrons moves almost along a straight line and their velocities and the angle ϑ_{12} vary little.

The smaller E, the greater is the area of the space in which inequality (1) is not fulfilled and the more durable (i.e. at great distances) is the substantial mutual repulsion of electrons significant and the more accurate is their escape into opposite

directions. As a result, the complementary angle of electrons escaping after ionization as $E \to 0$ approaches π in all cases.

The motion of the electrons is subject to the laws of quantum mechanics. When both electrons drift away to a sufficiently great distance from the ion and from each other, the interaction potential changes slowly and the examination of the problem is simplified, since the results of its solution by means of quantum and classical mechanics are identical. At low energies, the boundary between the region of space in which quantum mechanics must be applied and the region where classical mechanics can be used, as well as the notion itself in the "quantum-mechanical" region, are practically independent of E and remain nearly the same as when $E = 0$.

But the smaller is E the greater is the region in which inequality (1) is not fulfilled, and the energy distribution and the reciprocal angle ϑ_{12} of electrons vary.

Thus, at small values of E the energy and the complementary angular distribution of electrons are determined mainly by the region where the motion can be described by classical methods. For this reason, the set up of the threshold law can be divided into two parts. First, by solving the quantum-mechanical problem, we must determine the probabilities with which electrons with given velocities fly into region of classical motion. Then, considering these velocities and coordinates as initial values, we must solve the equation of classical mechanics and study the motion of electrons as $t \to \infty$. It is difficult to find an exact solution for the first part of the problem. However, in order to obtain certain formulas for the threshold behaviour with a precision to within constant factors it is sufficient to assume that the electrons fly into the region of classical motion with a smooth velocity and directional distribution.

It is not possible to solve all problems concerned with the threshold behaviour by using such assumptions; for example, one cannot find the angular distribution of escaping electrons with respect to the direction of motion of an incident electron. Since there are no foundations to assume that ionization will take place near the threshold only at a total moment $L = 0$, this distribution will not be isotropic and in order to find its form the problem must be solved in the "quantum-mechanical" region.

If $L \neq 0$, centrifugal terms $\sim r^{-2}$ appear in the equations of motion. These terms have a weak effect at great distances inasmuch as they decrease more rapidly than the Coulomb terms ($\sim r^{-1}$). Furthermore in this article we shall examine only such problems for which at small E substantial is mainly the interaction at great values of $\mathbf{r}_1$ and $\mathbf{r}_2$; for this reason we shall assume that

L = 0, knowing that at other, not too great*, values of L, we shall obtain the same result.

Let us now examine the mathematical derivations of Wannier's theory. Using a system of units in which the mass and the charge of an electron are equal to unity, the motion of electrons in the region where classical mechanics are applicable can be described by the following equations:

$$\frac{d^2\mathbf{r}_1}{dt^2} = -\frac{Z\mathbf{r}_1}{r_1^3} + \frac{\mathbf{r}_1 - \mathbf{r}_2}{|\mathbf{r}_1 - \mathbf{r}_2|^3};$$
$$\frac{d^2\mathbf{r}_2}{dt^2} = -\frac{Z\mathbf{r}_2}{r_2^3} + \frac{\mathbf{r}_2 - \mathbf{r}_1}{|\mathbf{r}_2 - \mathbf{r}_1|^3}. \qquad (2)$$

Here Z is the charge of the ion remaining after ionization. The mass of this ion is assumed to be infinite. Since the region examined here is located far beyond the limits of the ion, we assume that the ion creates a potential Zr^{-1}, which is independent of the position of its inner electrons.

Equations (2) have an important property which will be utilized to a significant extent further in this article. If $\mathbf{r}_i = \mathbf{f}_i(t)$ is the solution of (2), then for any value of constant B

$$\mathbf{r}_i = B^{-1}\,\mathbf{f}_i(B^{\frac{3}{2}}t) \qquad (3)$$

is also a solution of (2). This can be easily verified by substituting (3) into (2). The trajectories of these solutions are similar in form but differ in their scales and energies. If E is the energy of the initial solution, then the energy of (3) is equal to BE

For the ionization to take place it is necessary that an electron escape into the infinity with an energy in the 0 to E range. The smaller is E the smaller is the range of initial values corresponding to the ionization. To clarify the threshold behaviour of the ionization cross section, it is necessary to study the dependence of this range on E. One case leading to ionization can be easily found. This is the case when both electrons drift away from the ion along a single straight line in opposite directions, remaining all the time at equal distances from the ion and moving with identical velocity (in celestial mechanics, this case is known as the Lagrange colinear case):

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* The greater is L the smaller is the energy region in which the threshold laws examined in this article are valid.

$$\mathbf{r}_1 = -\mathbf{r}_2 \equiv \mathbf{r}. \tag{4}$$

Substituting (4) into (2) we obtain the equation

$$\frac{d^2r}{dt^2} = -\frac{Z-\frac{1}{4}}{r^2}, \tag{5}$$

in the solution of which r and t are linked by the relation

$$\sqrt{2E^3}\,\frac{t-t_0}{Z-\frac{1}{4}} = \sqrt{\rho(\rho+1)} - \frac{1}{2}\ln\left(2\sqrt{\rho(\rho+1)} + 2\rho + 1\right),$$
$$\rho \equiv Er\left(Z-\frac{1}{4}\right)^{-1}, \tag{6}$$

with t_0 and E as the integration constants. Further in this article we shall assume that $t_0 = 0$. In the region where $Er \ll Z$, formula (6) is reduced to

$$r^3 = \frac{9}{2}\left(Z-\frac{1}{4}\right)t^2 \tag{7}$$

and the motion does not depend on E. The smaller is E the larger is the space region where (7) is fulfilled, and at limit $E \to 0$ this equation is true in the entire space.

Ionization will take place not only under the initial conditions which lead to relations (4) and (6), but also under other closely related conditions. In order to study solutions close to (4) and (6) it is convenient to pass from the variable $\mathbf{r}_1$ and $\mathbf{r}_2$ to $\mathbf{r}$, $\Delta\mathbf{r}$, $\delta\mathbf{r}$:

$$\mathbf{r}_1 = \mathbf{r} + \Delta\mathbf{r} + \delta\mathbf{r};$$
$$\mathbf{r}_2 = -\mathbf{r} + \Delta\mathbf{r} + \delta\mathbf{r}, \tag{8}$$

where $\mathbf{r} = \frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_2)$, while $\Delta\mathbf{r} \parallel \mathbf{r}$ and $\delta\mathbf{r} \perp \mathbf{r}$ are components of $\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$. Substituting (8) into (2) we find that, when $L = 0$ and $|\Delta r| \ll r$, $|\delta r| \ll r$, a variable r value satisfies (5) and $\Delta\mathbf{r}$ and $\delta\mathbf{r}$ satisfy the equations

$$\frac{d^2\Delta r}{dt^2} = 2Z\frac{\Delta r}{r^3}; \qquad \frac{d^2\delta r}{dt^2} = -Z\frac{\delta r}{r^3}, \tag{9}$$

at the same time, the directions of these vectors do not vary with time. In the region $Er \ll Z$, where (7) serves as the solution of (5), Eq.(9) is reduced to

$$\frac{d^2\Delta r}{dt^2} = \frac{16Z}{9(4Z-1)} \cdot \frac{\Delta r}{t^2} \qquad \frac{d^2\delta r}{dt^2} = -\frac{8Z}{9(4Z-1)} \cdot \frac{\delta r}{t^2}, \tag{10}$$

the common solution of which are the following equations:

$$\Delta r = r\left(C_1 r^{-\frac{1}{4}-\frac{\mu}{2}} + C_2 r^{-\frac{1}{4}+\frac{\mu}{2}}\right); \tag{11}$$

$$\delta r = r\left(C_3 r^{-\frac{1}{4}-\frac{\nu}{2}} + C_4 r^{-\frac{1}{4}+\frac{\nu}{2}}\right); \tag{12}$$

$$\mu = \frac{1}{2}\sqrt{\frac{100Z-9}{4Z-1}}, \quad \nu = \frac{1}{2}\sqrt{\frac{4Z-9}{4Z-1}}. \tag{13}$$

Taking (7) into account, the independent variable $\underline{t}$ in (11) and (12) is replaced by $\underline{r}$.

When $Z \leqslant 2$, ν is imaginary and $C_3 = C^*$ are complex quantities. If $Z \geqslant 3$ these quantities are real,[4] but ν is always smaller than 1/2. Therefore, in the region where (12) is applicable the ratio $\delta r/r$ always decreases as $\underline{r}$ increases, i.e. the angle between the electrons approaches π. When Z is equal to 1 or 2, then, according to (12), $\delta r/r$ decreases proportionally to $r^{-\frac{1}{4}}$ and in view of the imaginary nature of ν it still oscillates near zero.

The quantity μ is greater than 5/2 for all values of Z. Therefore, as $\underline{r}$ increases the first term in expression (11) decreases while the second one increases. When $C_1 = 0$, the second term describes the case when both electrons escape from the atom simultaneously but with somewhat different velocities. This difference in velocities is proportional to C_2. When $C_2 = 0$, the first term describes the case when electrons do not escape from the atom simultaneously, but their velocities are such that the condition $r_1 = r_2$ is fulfilled far from the ion. The sum of both terms represents a general case.

Solutions (11) and (12) are applicable if $|\Delta r| \ll r$, $|\delta r| \ll r$. In most cases, after a collision both electrons escape from the atom with noticeably different velocities and the inequality $|\Delta r| \ll r$ is not fulfilled. However, we shall not consider such cases inasmuch as there is no ionization in such a situation. After a quantitative study of the equations of motion, Wannier found that ionization will take place at small values of E only in the case when the electron trajectories run through the region where (11) and (12) are applicable*. We shall not bring forth here the conclu-

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* In celestial mechanics, Sundman [9] has found a smilar rule, namely when $\underline{t}$ approaches the moment of general collision the configuration formed by the particles approximates (or comes close to) one of the two configurations characterizing the Lagrange colenear or equidistant solutions.

sion drawn by Wannier, but we shall merely point out that this conclusion is based mainly on two considerations. The inequality $|\Delta r| \ll r$ is fulfilled because, when $E \ll 1$ ionization will take place only when the electrons escape from the atom with velocities rather close to each other. Otherwise, the slower electron remains longer in the vicinity of the ion, shielding its charge for the faster electron and therefore more distant with time. As a result the kinetic energy of the faster electron, does not decrease to a sufficient extent as $t \to \infty$, i.e. it stays greater than E, and no ionization takes place.

If the condition $|\delta r| \ll r$ is not fulfilled at the origin of the trajectory the mutual repulsion of electrons will result in its fulfillment during further motion.

To find the threshold behaviour of the cross section it is necessary to determine how the energies and the complementary angle of electrons depend at infinity on C_1, C_2, C_3, C_4 under the initial conditions (11) and (12). Moreover, one must be aware of the probability distribution of electrons for these constants with which they escape from the region of "quantum-mechanical" motion and fly into the region where (11) and (12) are applicable. Since the "quantum-mechanical" region is spatially limited (its dimensions are of the order of several Bohr radii) and the motion does not depend on E when $Er \ll Z$ (i.e. E appears only in higher terms of the expansion in powers of E), we can assume that at small E values the electrons fly into the region where (11) and (12) are applicable with a smooth velocity and directional distribution which is independent of E. As a result, if we are interested only in the first term of the expansion in powers of E, the probability density of constants C_i may be considered as independent of E in the case of small values of E. This density is standarized for unity and therefore approaches zero at high value of C_i.

For small values of C_i, there is a linear dependence between the energies of electrons at infinity and C_1 and C_2 and between their complementary angle and C_3 and C_4. Using (3) we may determine how the region of C_i values, in which the indicated linear dependence takes place, varies, as E becomes smaller.

According to (3), the dimensions of similar trajectories are inversely proportional to E. We shall obtain for various values of E similar trajectories if, in the initial conditions (11) and (12), we vary C_2 proportionally to $E^{-\frac{1}{4}+\frac{\mu}{2}}$ and C_1, C_3 and C_4 proportionally to $E^{-\frac{1}{4}-\frac{\mu}{2}}$ $E^{-\frac{1}{4}-\frac{\nu}{2}}$ and $E^{-\frac{1}{4}+\frac{\nu}{2}}$ respectively. Subjecting to such a transformation the trajectories, of which the energies and the angles depend linearly on C_i, we shall again obtain trajectories with linear dependence. Therefore, when E decreases,

the region of linearity with respect to C_2 will decrease proportionally to $E^{-\frac{1}{4}+\frac{\mu}{2}}$ while the regions of linearity with respect to C_1, C_3, C_4 will increase proportionally to the remaining above-mentioned powers of E. As a result, when E is sufficiently small, the dependence on C_1, C_3, C_4 will be linear (and the smaller is E the less so) in the entire region where the probability density of these constants is somewhat different from zero. This is why for small E the energies of escaping electrons are determined only by the one constant C_2.

The direct finding of this dependence is made difficult by the fact that, in the cases when the energies of electrons at infinity differ greatly, Eqs.(2) can be linearized with respect to C_2 only in the initial portion of the trajectory, where (7), (11) and (12) are valid. Therefore, we shall subsequently determine the energy distribution of electrons by numerical integration. However, even if the form of this distribution is unknown, we can find its dependence on the total energy E by using (3).

Ionization will take place only in the terminal range of C_2 values. According to (3) and (11), the length of this range decreases proportionally to $E^{-\frac{1}{4}+\frac{\mu}{2}}$ with decreasing E and will be small at small values of E. —— The probability density of C_2 will be a smooth function of C_2 insofar as, according to (7) and (11), in the case of fixed values of C_1, and r, C_2 is proportional to the difference in velocities of both electrons. Since we are interested only in the first term of the expansion in powers of E, this probability density of C_2 can be considered as being constant in the ionization range. Then, the total ionization cross section is simply proportional to the length of the range of C_2 values leading to ionization:

$$\sigma_{\text{ioniz}} \sim E^{\frac{\mu}{2}-\frac{1}{4}}, \qquad (14)$$

which is precisely the result obtained by Wannier. If Z = 1, then, according to (13) and (14), $\sigma_{\text{ioniz}} \sim E^{1.127}$. The greater is Z the closer is this dependence to a linear one.

Summerizing, it can be stated that the Wannier's theory is based on the following four considerations:

1. At small values of E, the energy dependence of ionization cross sections is determined mainly by the region where particles are far from each other and their interaction potentials vary slowly, and therefore the motion is subject to the laws of classical mechanics inasmuch as the results of quantum and classical mechanics are identical in this case.

2. Electrons enter this region with a smooth velocity and

directional distribution which for small values of E can be principal term of the expansion is the only one of interest, if considered as independent of E.

3. At small values of E, only those trajectories lead to ionization which pass in their initial portion, through the region where linearized solution of (11) and (12) are applicable.

4. The law of similarity (3) can be used to find the energy dependence of ionization cross sections.

COMPLEMENTARY ANGLE AND ENERGY DISTRIBUTION OF ELECTRONS AFTER IONIZATION

If $C_3 = C_4 = 0$ the electrons escape in opposite directions and the angle ϑ_{12} between their radii at infinity is equal to π. When C_3 and C_4 are small, the difference $\vartheta_{12} - \pi$ is small and depends linearly on C_3 and C_4 (if C_1 and C_2 are fixed), since the equation of motion can be linearized with respect to δr (independently of the quantity Δr). In the linearity region, at fixed values of C_3 and C_4, the difference $\vartheta_{12} - \pi$ decreases, with decreasing E. The term with C_3 decreases proportionally to $E^{\frac{1}{4}+\frac{\nu}{2}}$, and the term C_4 proportionally to $E^{\frac{1}{4}-\frac{\nu}{2}}$. If $Z \geqslant 3$, then $0 < \nu < \frac{1}{2}$ and at small values of E, when the more rapidly decreasing term C_3 can be disregarded $\vartheta_{12} - \pi \sim C_4 E^{\frac{1}{4}-\frac{\nu}{2}}$. If Z = 1 or 2, then ν is an imaginary value and $\vartheta_{12} - \pi$ decreases proportionally to $E^{\frac{1}{4}}$, oscillating through zero in view of the terms $E^{\pm i\frac{|\nu|}{2}}$.

For constant C_i form of the complementary angle distribution is determined by the probability densities. Since at sufficiently small energies the dependence of the difference $\vartheta_{12} - \pi$ on C_3 and C_4 will be linear in most cases, the form of the angular distribution will not change with decreasing E but will only become proportional to $E^{\frac{1}{4}-\frac{\nu}{2}}$, provided $Z \geqslant 3$, or proportional to $E^{\frac{1}{4}}$ when Z = 1 or 2. In the latter case the oscillating terms $E^{\pm i\frac{|\nu|}{2}}$ will not cause fluctuations in the angular distribution inasmuch as they are multiplied by C_3 and C_4, which are also complex and whose phases undergo random variations.

As a result, by studying the motion in the region where classical mechanics are applicable it is possible to determine how the complementary angular distribution narrows down with an increase in E, but in order to find the form of this distribution it is also necessary to solve the problem in the "quantum-mechanical" region.

On the other hand, the distribution of energy among electrons can be found by solving only the equation of classical mechanics. As was shown earlier, only the one constant C_2, the probability density of which can be considered as constant, determines the energy distribution at small value of E. Therefore, Eq.(2) must be integrated at a certain fixed energy E, at the initial conditions (11) and (12), at $C_1 = C_3 = C_4 = 0$ and at different values of C_2, and the energy of one of the electrons (for example, the first one) must be determined at infinity $E_1(\infty)$ as a function of C_2. In other words, we must construct a function of $C_2 = f(\varepsilon)$ $\left(\varepsilon \equiv \frac{E_1(\infty)}{E}\right)$, the derivative of which $\frac{df(\varepsilon)}{d\varepsilon}$ in the range $0 \leqslant \varepsilon \leqslant 1$ is proportional to the probability that the first electron escapes after ionization with the energy $E_1(\infty) = \varepsilon E$ and consequently, yields after standardization the probability density of the relative energy distribution.

It follows from the law of similarity (3) that, at different E values, functions $f(\varepsilon)$ differ only by their constant factor and therefore for small values of E the form of energy distribution is independent of E. To find the form of this distribution, Eqs.(2) were numerically integrated on a BESM-2M electronic computer.

When $C_3 = C_4 = 0$, the motion takes place along a single straight line and Eqs.(2) are reduced to

$$\ddot{r}_1 = -\frac{Z}{r_1^2} + \frac{1}{(r_1 + r_2)^2};$$
$$\ddot{r}_2 = -\frac{Z}{r_2^2} + \frac{1}{(r_1 + r_2)^2} \qquad (15)$$

and when $C_1 = 0$, the initial values of (11), (12), are expressed in the form

$$r_{1,2} = r \pm C_2 r^{\frac{3}{4}+\frac{\mu}{2}};$$
$$\dot{r}_{1,2} = \left[1 \pm C_2\left(\frac{3}{4} + \frac{\mu}{2}\right) r^{-\frac{1}{4}+\frac{\mu}{2}}\right]\dot{r}, \qquad (16)$$

where

$$\dot{r} = \sqrt{E + 2\frac{Z - \frac{1}{4}}{r}}. \qquad (17)$$

The numerical integration was carried out by Runge-Kutta's fourth order method with Merson's [10] modification. The integration step was automatically selected in such a way that the error resulting from disregarding higher expansion terms in the integration formula do not exceed $0.5 \cdot 10^{-5}$. The integration was carried out for E = 1, starting with r = 0.001 and ending with $r_{min} \geqslant 10^4$, where r_{min} is the distance from the nearest electron to the ion.

The dependence of C_2 on ε is shown in Figures 1 and 2. Within the limits $Z \to \infty$ function $C_2 = f(\varepsilon)$ must be precisely linear, since in that case the interaction between electrons is negligibly small by comparison with their interaction with the ion. Therefore, the energies of both electrons are preserved separately. In this case, the dependence of electron energy at infinity on C_2 is linear, inasmuch as according to (16) in the initial portion of the trajectory the small values of C_2 will cause small and linear electron energy deviations with respect to C_2 from $\frac{E}{2}$.

As may be seen from Figs. 1 and 2, functions $C_2 = f(\varepsilon)$ do not practically differ from straight lines even when $Z \neq \infty$. Therefore, the probability density of relative energy distribution in the ionization range is practically constant for any values of Z. Insignificant deviations from a constant value increase as Z decreases. These deviations are zero when $\varepsilon = 0.5$ and reach maximum values when $\varepsilon = 0$ and $\varepsilon = 1$. But even then, when $Z = 1$, these deviations are smaller than 1%.

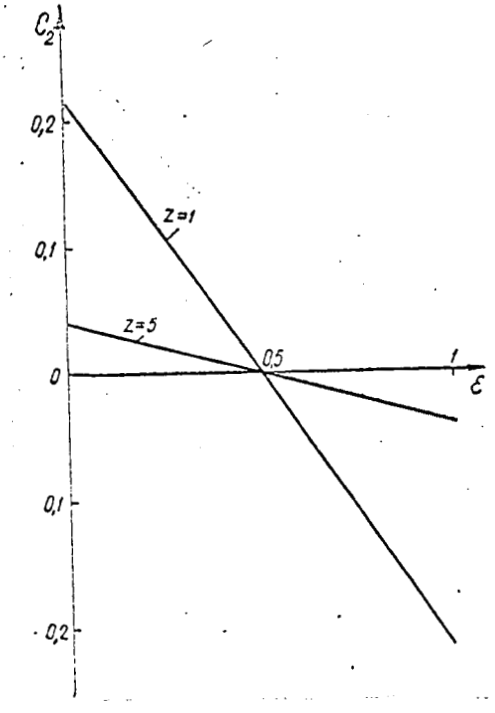

Fig.1.
Dependence of C_2 on

when $Z = 1$ and $Z = 5$

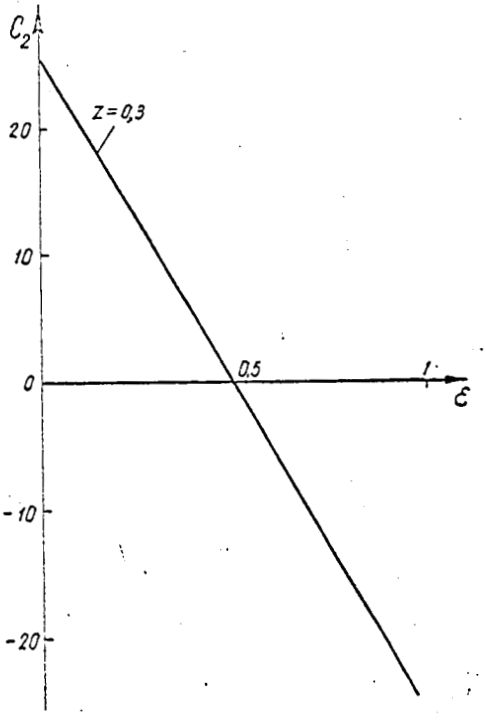

Fig.2.
Dependence of C_2 on ε when

$Z = 0.3$.

Figure 2 shows the dependence of C_2 on ε found formally by solving the problem for $Z = 0.3$. It was found that in this case

the change in the probability density is greater than for Z = 1, but even then the changes are insignificant and are less than 2%.

For small E we may find by the Wannier's method not only the energy distribution of electrons escaping after ionization but determine also the probabilities of excitation of highly excited levels. For this purpose, it is necessary to calculate $f(\varepsilon)$ for negative values of ε. If for E = 1 $C_2 = f(E_1(\infty))$, then according to (3) and (11) for other energies $C_2 = E^{\frac{\mu}{2}-\frac{1}{4}} f(E_1(\infty)/E)$. The probability of excitation of the n-th Bohr level with such a low energy E_n, that the motion can be considered in a quasiclassical manner, is then proportional to

$$E^{\frac{\mu}{2}-\frac{1}{4}} [f(E_n/E) - f(E_{n+1}/E)] \approx E^{\frac{\mu}{2}-\frac{5}{4}} (E_{n+1} - E_n) |f'(E_n/E)|,$$

where $f'(\varepsilon) = \frac{df(\varepsilon)}{d\varepsilon}$. Let us note that the total ionization cross section is proportional to $E^{\frac{\mu}{2}-\frac{1}{4}}\left[f(0) - f\left(\frac{1}{2}\right)\right]$ with the same proportionality factor. Figure 3 shows $f(\varepsilon)$ found numerically for Z = 1 and negative ε values. As may be seen, function $f(\varepsilon)$ does not deviate much from a linear dependence and its derivative $f'(\varepsilon)$ is almost constant. Therefore, if E_n is of the same order or smaller than E the probability of excitation of the n-th level is simply proportional to the distance between neighboring levels $E_{n+1} - E_n$ and varies slowly with energy variation, namely as $E^{\frac{\mu}{2}-\frac{5}{4}}$ (i.e. $E^{0.127\ldots}$ when Z = 1). The deviations of $f(\varepsilon)$ from linearity increase as $|\varepsilon|$ increases. When $|\varepsilon| \gg 1$ $f(\varepsilon)$ must increase as $|\varepsilon|^{\frac{\mu}{2}-\frac{1}{4}}$ (i.e. $\sim |\varepsilon|^{1,127\ldots}$ when Z = 1) since when $E_n \gg E$, the probability of excitation must be weakly dependent on E.

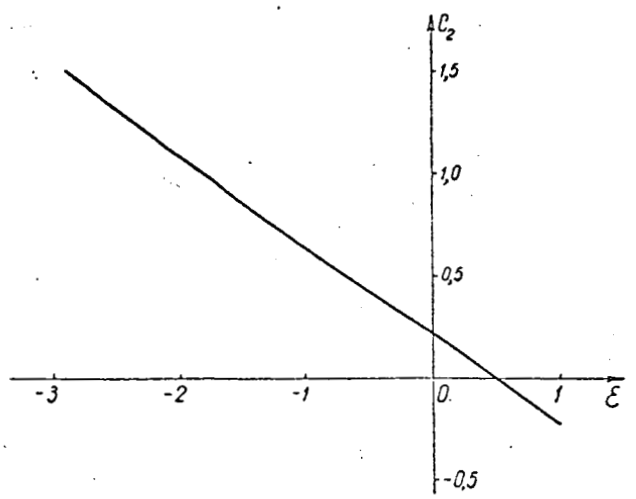

Fig. 3. Dependence of C_2 on ε in ionization and excitation ranges with Z = 1.

The significant feature of Wannier's theory is the fact that electrons escape from the ion in opposite direction as a result of mutual repulsion, i.e. as the electrons drift farther away from the ion ϑ_{12} approaches π and $\delta r/r$ approaches zero. Therefore the laws of threshold behavior thus obtained are applicable only when E values are so small that, in the region $|U(r_1, r_2)| \gg E$, where the motion does not depend on E, $\delta r/r$ has time to decrease sufficiently, i.e., so that a linearized solution of (12) may be applicable for most trajectories of interest to us.

To determine how fast $\delta r/r$ decreases in practice we have investigated equations of motion (2) for Z = 1 values when E = L = 0 and $r_1 = r_2$ all the time by numerically integrating the cases of such initial.

The dependence $\psi \equiv \frac{1}{2}(\vartheta_{12} - \pi)$ or $\frac{r}{r_0}$ on $\frac{r}{r_0}$ thus obtained is shown in Figure 4. Here, $\underline{r}$ is the distance between the electron and the ion and r_0 is one of the values of $\underline{r}$ at which $\dot{\vartheta}_{12} = 0$. According to (3), when E = 0, the trajectories with different r_0 values are similar in shape but their dimensions are proportional to r_0. This is why the trajectories with different initial conditions give in Fig.4 a one-parameter family of curves $\psi\left(\frac{r}{r_0}\right)$ with different heights of $\psi(1)$ peaks when $r = r_0$. $\psi < \psi_{max} = \arccos\frac{1}{4}$ always takes place. Otherwise the energy of repulsion between electrons is greater than the energy of their attraction to the ion, which is impossible when E = 0. The lower curves in Fig.4 are close to a linearized soluton of (12) which, substituting C_3 and C_4 by other constants A and r_0, can be written in the form:

$$\psi = A\left(\frac{r}{r_0}\right)^{-\frac{1}{4}}\left|\cos\left(\frac{1}{4}\sqrt{\frac{5}{3}}\ln\frac{r}{r_0} - \operatorname{arctg}\sqrt{\frac{3}{5}}\right)\right|. \qquad (18)$$

The behavior of ψ in (18) when $\underline{r}$ increases is determined mainly by the decreasing term $r^{-\frac{1}{4}}$. The cosine agreement varies slowly and increases by $\frac{\pi}{2}$ when $\underline{r}$ rises 130 times. Since such high values of $\frac{r}{r_0}$ are not shown in Fig.4 for the lower curves, only the diminishing but not the complementary oscillatory character of these curves can be seen. According to Fig.4, the departures of the solutions from (18) increase as $\psi(1)$ increases and the oscillations become more rapid. The amplitude of oscillations decreases as $\underline{r}$ increases for all $\psi(1)$ (every successive peak is

lower than the preceeding one*). Therefore, at sufficiently great values of r, the motion takes place according to linearized solutions. However, the approximation to these solutions is slow, particularly if $\psi(1)$ is close to ψ_{max}. This fact may limit the region of applicability of the above-mentioned threshold laws to very low energies.

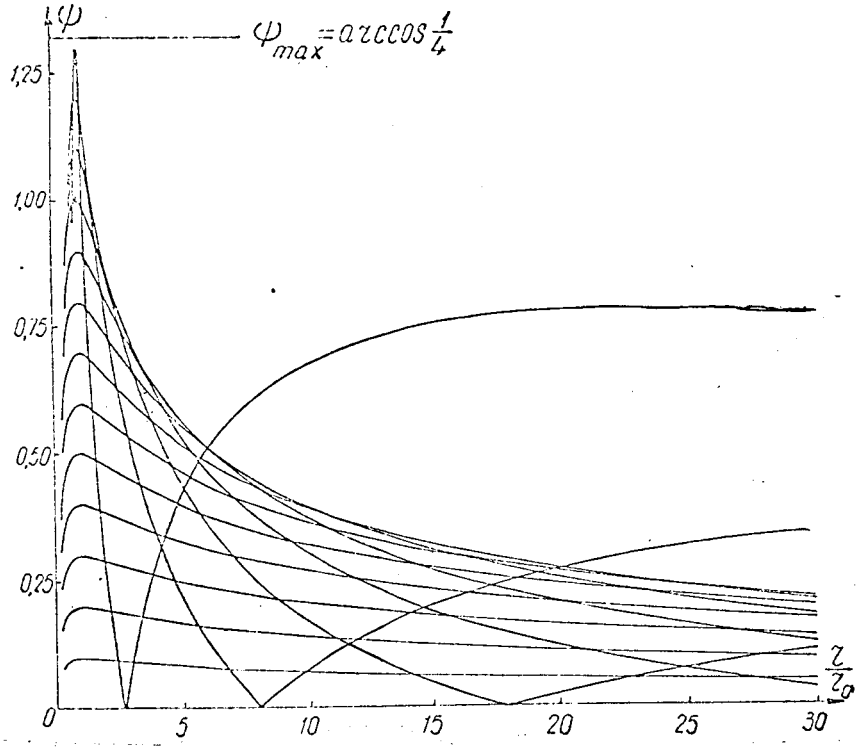

Fig. 4.

Dependence of $\psi \equiv \frac{1}{2}(\vartheta_{12} - \pi)$ on $\frac{r}{r_0}$.

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* Every curve oscillates in an infinite-to-one manner. In order to determine the dependence of these oscillations on $\psi(1)$, it is sufficient to know the shape of the curves between two adjacent peaks. Postulating the height of the new peak again equal to $\psi(1)$ and its position being r_0, we can find the height and the position of the next peak, etc.,

ENERGY DISTRIBUTION FOR THE CASE WITH A POTENTIAL $\sim r^{-2}$

In order to understand the reasons responsible for the practically linear dependence of C_2 on ε, it is interesting to ascertain whether such a dependence is characteristic only for a Coulomb field or whether it is observed also in other cases. This is why we shall study in this section the problem of the case when the interaction forces are inversely proportional to the cubes of the distances. In this case, the problem of motion along a single straight line ($C_3 = C_4 = 0$) can be solved analytically, as was shown by Jacobi [8]. If the vectors r_1 and r_2 run in opposite directions, the interaction potential has the form:

$$U = -\left[\frac{Z}{r_1^2} + \frac{Z}{r_2^2} - \frac{1}{(r_1 + r_2)^2}\right]. \tag{19}$$

For the equation of motion

$$\ddot{r}_1 = -\frac{\partial U}{\partial r_1}; \quad \ddot{r}_2 = -\frac{\partial U}{\partial r_2} \tag{20}$$

similarly to (7) and (11), we find the solution

$$r_1 = r_2 = (8Z - 1)^{\frac{1}{4}} t^{\frac{1}{2}} \tag{21}$$

and the solutions close to the latter

$$r_{1,2} = (8Z - 1)^{\frac{1}{4}} t^{\frac{1}{2}} [1 \pm (C_1 t^{-\mu} + C_2 t^{\mu})]. \tag{22}$$

At the same time

$$\mu = \frac{1}{2} \sqrt{\frac{32Z - 1}{8Z - 1}}. \tag{23}$$

The solutions (22) satisfy (20) when

$$|r_1 - r_2| \ll r_1; \qquad Er_1^2 \ll Z. \tag{24}$$

Because of the last inequality, when $E \neq 0$, the solutions satisfy formula (22) only near the origin of coordinates. We must ascertain how the electron energies depend on C_2 as $t \to \infty$, if formula (22) with $C_1 = 0$ is valid for small values of t.

Multiplying the first equation in (20) by r_1 and the second one by r_2, summing them up and still adding to them the following equations

$$2(\dot{r}_1^2 + \dot{r}_2^2) = 4E - 4U, \tag{25}$$

we obtain

$$\frac{d^2}{dt^2}(r_1^2 + r_2^2) = 4E, \tag{26}$$

inasmuch as the sum of the terms containing U is zero because of the uniformity of potentials. Passing in (26) from r_1, and r_2 to the new variable ρ and ϕ

$$r_1 = \rho \sin\varphi \quad \text{and} \quad r_2 = \rho\cos\varphi, \tag{27}$$

we obtain the equation

$$\frac{d^2\rho^2}{dt^2} = 4E \tag{28}$$

with the solution

$$\rho^2 = 2t\,[\,Et + (8Z-1)^{\frac{1}{2}}\,], \tag{29}$$

which, when conditions (24) are met, corresponds to (22) with $C_1 = 0$.

In the solution (29) ρ does not depend on C_2. Thus, we find that only ϕ depends on C_2. Substituting (27) and (29) into (25) we obtain an equation for the determination of $\phi(t)$:

$$\rho^4\dot{\varphi}^2 = 2\Delta(\varphi) - 8Z + 1; \tag{30}$$

$$\Delta(\varphi) \equiv -\rho^2 U = Z\sin^{-2}\varphi + Z\cos^{-2}\varphi - (\sin\varphi + \cos\varphi)^{-2}. \tag{31}$$

Eq.(30) is integrated in quadratures. At initial conditions (22) with $C_1 = 0$, the solution of this equation is the following equality:

$$\int_{\frac{\pi}{4} + C_2 t_0^{\mu}}^{\varphi} \frac{d\varphi}{\sqrt{2\Delta(\varphi) - 8Z + 1}} = \int_{t_0}^{t} \frac{dt}{2t\,[Et + (8Z-1)^{\frac{1}{2}}]}. \tag{32}$$

We must pass in both parts of equality (32) to the limit $t_0 \to 0$. From (32) we obtain the dependence between C_2 and the

energy of the first electron at infinity in the case of ionization:

$$(8Z-1)^{\frac{\mu}{2}} C_2 = E^{\mu}\left(\varepsilon - \frac{1}{2}\right)\Im(\varepsilon, Z), \tag{33}$$

where

$$\Im(\varepsilon, Z) = \left(\frac{y+1}{2}\right)^{\mu-1}\left[\frac{2\left(1-\frac{1}{32Z}\right)}{1-\frac{\beta}{16Z}+\sqrt{\left(1-\frac{1}{32Z}\right)\left(1-\frac{\beta^2}{8Z}\right)}}\right]^{\frac{1}{2}}$$
$$\times\left[\frac{1-\frac{\beta}{8Z}+\sqrt{\left(1-\frac{1}{8Z}\right)\left(1-\frac{\beta^2}{8Z}\right)}}{1-\frac{1}{16Z}+\sqrt{\left(1-\frac{1}{8Z}\right)\left(1-\frac{1}{32Z}\right)}}\right]^{\mu}; \tag{34}$$
$$y \equiv 2\sqrt{\varepsilon(1-\varepsilon)}; \beta = \frac{y}{1+y}.$$

Similarly to the Coulomb case, it follows from (33) that the C_2 range in which ionization can take place with decrease of E decreases proportionately to E^{μ} and that the form (shape) of the probability density of the relative energy distribution does not depend on E.

The departure from linearity of the dependence of C_2 on ε is determined by the factor $\Im(\varepsilon, Z)$ in (33). According to (34), $\Im(\varepsilon, Z)$ depends on ε. However, as can be seen from Figure 5, this dependence is in fact extremely weak. When $Z = \infty$ $\Im(\varepsilon, \infty) = 1$ and it does not depend on ε. When $Z = 1$ $\Im(\varepsilon, 1)$ varies from unity to 0.9947, and when Z = 0.125 it varies from 1 to 0.9510. If $Z < 1/8$, then μ is an imaginary value and our analysis is not applicable.

Thus, as in the Coulomb case, the probability density of the relative energy distribution $\sim \frac{dC_2}{d\varepsilon}$ is practically also constant when $U \sim \frac{1}{r^2}$.

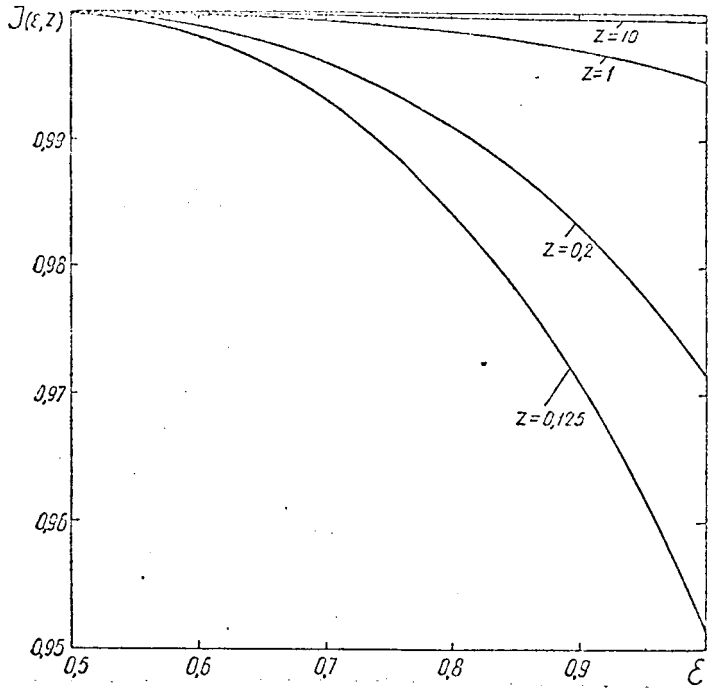

Fig.5.

Dependence (34) of $\mathfrak{J}$ on ε and Z.

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